Benzenesulfonic acid, 2-chloro-5-nitro-, sodium salt 946-30-5 | DTXSID4061339

340-30-3 D 1701D400 1333

Model Performance

Mode	Data

Weighted KNN model

5-fold CV (75%)		Training (Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE	
0.89	0.25	0.88	0.26	0.75	0.38	

Model Results

Predicted value: 4.47 days

Global applicability domain: Outside

Local applicability domain index: 2.78e-01

Confidence level: 8.05e-01

Nearest Neighbors from the Training Set

Image not found

1-Methyl-2-propylbenzene

Measured: 12.5 Predicted: 3.17

Image not found

3-Ethyltoluene

Measured: 12.5 Predicted: 3.26

Image not found

Propylbenzene

Measured: 24.3 Predicted: 4.02

Image not found

Tetradeca-1,13-diene

Measured: 367 Predicted: 8.69

Image not found

1-Ethyl-2-methylbenzene

Measured: 24.3 Predicted: 3.88